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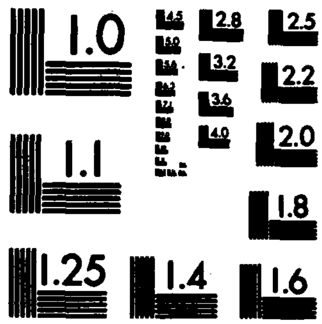

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During this period research was continued on the development and application of numerical methods for singularly-perturbed (or stiff) boundary value problems for ordinary differential equations and initial-boundary value problems for partial differential equations. The author concentrated most heavily on extensions to the adaptive finite element methods for partial differential equations. In particular, the stability of several mesh moving schemes was analyzed and local refinement techniques developed. The author also has some encouraging preliminary results on mesh moving methods in two dimensions.

The investigators are applying their methods to several interesting physical problems, such as: elastic-plastic solids, combustion, and a nonlinear Schrodinger equation which exhibits self focusing.

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INTERIM SCIENTIFIC REPORT

Air Force Office of Scientific Research Grant AFOSR-80-0192

Period:	1 June 1983 through 31 May 1984
Title of Research:	Numerical Methods for Singularly Perturbed Differential Equations with Applications
Principal Investigator:	Joseph E. Flaherty

Department of Computer Science
Rensselaer Polytechnic Institute
Troy, New York 12181

ABSTRACT

During the period covered by this report we continued our research on the development and application of numerical methods for singularly-perturbed (or stiff) boundary value problems for ordinary differential equations and initial-boundary value problems for partial differential equations. We concentrated most heavily on extensions to our adaptive finite element methods for partial differential equations. In particular, we analyzed the stability of several mesh moving schemes and developed local refinement techniques. We also have some encouraging preliminary results on mesh moving methods in two dimensions.

We are applying our methods to several interesting physical problems, such as, elastic-plastic solids, combustion, and a nonlinear Schrodinger equation which exhibits self focusing.

1. Progress and Status of the Research on Numerical Methods for Singularly-Perturbed Differential Equations

During the period covered by this report we continued our research on the development and application of numerical methods for singularly-perturbed ordinary and partial differential equations. We concentrated on partial differential equations, however, two of our papers [2,3][1] on numerical methods for singularly-perturbed two-point boundary value problems were accepted for publication.

Flaherty and several graduate students have been continuing their reserach on adaptive finite element methods for partial differential equations. Their findings on one-dimensional moving grid schemes for parabolic problems appeared in Adaptive Computational Methods for Partial Differential Equations[1], which was published by SIAM. Flaherty is one of the editors of these proceedings and J. M. Coyle, one of the authors of [1], is a graduate student who is being supported by this grant.

Reference [1] contains several applications, including a focusing problem for the nonlinear Schrodinger equation. This problem describes the self-focusing of a laser beam in a medium with a nonlinear index of refraction and it is being done in collaboration with Professor A. C. Newell of the University of Arizona. It is a difficult numerical problem because the amplitude of the solution becomes infinite as focusing occurs. Our adaptive finite element code appears to be able to cope with this difficulty and is giving

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[1] See the list of publications and abstracts at the end of this report.

very good results. We will discuss the physical and additional computational aspects of this problem in a forthcoming paper by Coyle, Flaherty and Newell [11].

Drew and Flaherty created a model for shear band instabilities that involves the rapid shearing of a slab of a visco-elastic material with small viscosity. They used the adaptive finite element code of [1] to solve their model and illustrated several possible mechanisms for shear band formations. Some of their preliminary findings will appear in the proceedings of the conference on Phase Transformations and Material Instabilities in Solids [4]. They are extending their model to include visco-plastic materials and a more accurate energy equation. In a somewhat related study, Slemrod and Flaherty considered appropriate finite difference schemes for phase transitions involving van der Waals fluids. They submitted their initial findings to Res Mechanica [6], but are anxious to conduct further studies using their finite difference schemes in an adaptive setting.

In reference [1] we showed that many mesh equidistribution schemes lead to unstable differential equations for mesh velocities when they are applied to dissipative partial differential equations. We have continued this study and are now able to categorize the stability or instability of a large class of mesh equidistribution schemes for the finite difference or finite element solution of partial differential equations. Our findings have been incorporated into a paper by Coyle, Flaherty and Ludwig which we submitted to the Journal of Computational Physics [7].

Flaherty and graduate students Adjerid, Arney, Coyle, Hayes and Moore have been studying several improvements and additions to the adaptive finite

element code of [1]. For one-dimensional problems, J. M. Coyle has been examining mesh adaptation and equidistribtuion strategies and has also been developing a p-version adaptive finite element code. P. Moore has implemented procedures that recursively perform local time and spatial step refinements in regions of high error. This work will appear in the proceedings of the Conference on Accuracy Estimates and Adaptive Refinements in Finite Element Computations [5] which will be held in Lisbon in June 1984. A second report on some improvements to our local refinement method is being prepared by Moore and Flaherty and will be submitted for publication in the Proceedings of the Second Army Conference on Applied Mathematics and Computing [9].

S. Adjerid has been working on adaptive procedures for a posteriori error estimation and mesh refinement for moving finite element methods. His work on one-dimensional problems was presented at the meeting of the Northeast Applied Mathematics Consortium and a paper on it is being prepared for publication in the SIAM Journal on Numerical Analysis [10].

For two-dimensional problems, Maj. D. C. Arney is implementing adaptive mesh moving and equidistribution procedures and Cpt. J. Hayes has implemented a two- and three-dimensional graphics package to assist him with pre and post processing tasks. Major Arney and Captain Hayes are U. S. Army officers who are on educational leave from the U. S. Military Academy. Captain Hayes just completed his M. S. degree in Applied Mathematics and is returning to West Point. Major Arney is a Ph.D. student under Flaherty's direction.

A paper on Arney's work on two-dimensional mesh moving schemes is currently in its final stages of preparation [9]. This technique uses the

notion of regions of significant error to control the motion of the mesh and, unlike many other two-dimensional mesh moving schemes, it has no problem dependent parameters.

2. Interactions

Professor Flaherty and graduate students supported by this grant lectured and/or visited the following conferences and organizations during the period covered by this report:

J. E. Flaherty presented a contributed paper on "Adaptive Finite Element Methods for Wave Propagation and Impact in Rods" at the SIAM National Meeting, Denver, 6-8 June 1983.

J. E. Flaherty presented a lecture on "Large Scale Computation" to representatives of the U. S. Air Force Seven-Man Group on Research in the Twenty-First Century at R.P.I. on 13 July 1983. He also attended a briefing on 5 June 1984 at Hanscom Air Force Base by Col. M. F. Burke on the findings of this group.

J. E. Flaherty presented a lecture on "Adaptive Finite Element Methods and Equidistribution Strategies for Parabolic Partial Differential Equations" at the University of Maryland on 22 September 1983. He also consulted with Professors S. Antman, I. Babuska and M. Vogelius of the University of Maryland and Dr. M. Bieterman of the National Institutes of Health as part of this trip.

J. E. Flaherty presented a lecture on "Adaptive Finite Element Methods and the Numerical Solution of Shear Band Problems" at the Conference on Phase Transitions and Material Instabilities in Solids, Univeristy of Wisconsin, Madison, 11-13 October 1983.

J. E. Flaherty attended the SIAM Fall meeting at the Omni International Hotel, Norfolk. He consulted with several individuals.

J. E. Flaherty attended the AFOSR Supercomputing Meeting at the Air Force Weapons Laboratory, Albuquerque, 4-6 April 1984. He also lectured on "Adaptive Finite Element Methods and Equidistribution Strategies for Partial Differential Equations" at the University of New Mexico on 6 April 1984 as part of this trip.

S. Adjerid lectured on "Moving Finite Element Methods with Error Estimation for Time Dependent Partial Differential Equations" at the meeting of the Northeast Applied Mathematics Consortium, Clarkson College of Technology, Potsdam, 20-21 May 1984.

J. E. Flaherty lectured on "An Adaptive Local Refinement Finite Element Method for Parabolic Partial Differential Equations" at the Second Army Conference on Applied Mathematics and Computing, R.P.I., 22-25 May 1984. He also helped organize this conference with D. A. Drew, S. L. Pu and J. D. Vasilakis.

3. List of Publications and Manuscripts in Preparation

Publications

1. J. E. Flaherty, J. M. Coyle, R. Ludwig and S. F. Davis, "Adaptive Finite Element Methods for Parabolic Partial Differential Equations," in I. Babuska, J. Chandra and J. E. Flaherty (Eds.), Adaptive Computational Methods for Partial Differential Equations, pp. 144-164, SIAM, Philadelphia, 1983.

In Press

2. R. E. O'Malley, Jr. and J. E. Flaherty, "On the Numerical Solution of Singularly-Perturbed Boundary Value Problems", to appear in Trans. Tenth IMACS World Conf., Montreal, Que., August 1982.

3. J. E. Flaherty and R. E. O'Malley, Jr., "Numerical Methods for Stiff Systems of Two-Point Boundary Value Problems", NASA Contractor Report 166115, NASA Langley Research Center, Hampton, VA., April 1983. Also, to appear in SIAM J. Sci. and Stat. Comput., December 1984.

4. D. A. Drew and J. E. Flaherty, "Adaptive Finite Element Methods and the Numerical Solution of Shear Band Problems", to appear in M. Gurtin (Ed.) Phase Transitions and Material Instabilities in Solids, Academic Press, New York, 1984.

5. J. E. Flaherty and P. K. Moore, "An Adaptive Local Refinement Element Method for Parabolic Partial Differential Equations", to appear in Proc. Conf. Accuracy Estimates and Adaptive Refinements in Finite Element Computations, Lisbon, June 1984.

6. M. Slemrod and J. E. Flaherty, "Numerical Integration of a Riemann Problem for a van der Waals Fluid", submitted to Res. Mechanica, April 1984.

7. J. M. Coyle, J. E. Flaherty and R. Ludwig, "On the Stability of Mesh Equidistribtuion Strategies for Time Dependent Partial Differential Equations", submitted to J. Comp. Phys., May 1984.

In Preparation

8. J. E. Flaherty and P. K. Moore, "On Local Refinement Finite Element Methods for Time Dependent Partial Differential Equations", to be submitted to Proc. Second Army Conf. on Appl. Maths. and Comput., R.P.I., May 1984.

9. D. C. Arney and J. E. Flaherty, "A Mesh Moving Technique for Time Dependent Partial Differential Equations in Two-Space Dimensions", to be submitted to Proc. Second Army Conf. on Appl. Maths. and Comput., R.P.I., May 1984.

10. S. Adjerid and J. E. Flaherty, "A Moving Finite Element Method for Time Dependent Partial Differential Equations with Error Estimation and Refinement", to be submitted to SIAM J. Numer. Anal.

11. J. M. Coyle, J. E. Flaherty and A. C. Newell, "Focusing Problems for Damped and Undamped Nonlinear Schrodinger Equation", in preparation for Physica D.

ADAPTIVE FINITE ELEMENT METHODS

FOR PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS

Joseph E. Flaherty, J. Michael Coyle, Raymond Ludwig
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12181

and

Stephen F. Davis
Institute for Computer Applications in Science and Engineering
NASA Langley Research Center
Hampton, Virginia 23556

ABSTRACT

We discuss a finite element method for solving initial-boundary value problems for vector systems of partial differential equations in one space dimension and time. The method automatically adjusts the computational mesh as the solution evolves in time so as to approximately minimize the local discretization error. We are thus able to calculate accurate solutions with fewer elements than would be necessary with a uniform mesh.

Our overall method contains two distinct steps: a solution step and a mesh selection step. We solve the partial differential equations using a finite element-Galerkin method on trapezoidal space-time-elements with either piecewise linear or cubic Hermite polynomial approximations. A variety of mesh selection strategies are discussed and analyzed. Results are presented for several computational examples.

In Adaptive Computational Methods for Partial Differential Equations, I. Babuska, J. Chandra, and J. E. Flaherty (Eds.), pp 144-164, SIAM, Philadelphia 1983.

ON THE NUMERICAL SOLUTION OF SINGULARLY-PERTURBED VECTOR BOUNDARY VALUE PROBLEMS

by

Robert E. O'Malley, Jr.

and

Joseph E. Flaherty
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12181 USA

ABSTRACT

Numerical procedures are developed for constructing asymptotic solutions of certain nonlinear singularly-perturbed vector two-point boundary value problems having boundary layers at one or both end points. The asymptotic approximations are generated numerically and can either be used as is or to furnish a two-point boundary value code (e.g., COLSYS) with an initial approximation and a nonuniform computational mesh. The procedures are applied to a model problem that indicates the possibility of multiple solutions and problems involving the deformation of a thin nonlinear elastic beam resting on a nonlinear elastic foundation.

To appear in Trans. Tenth IMACS World Conf., Montreal Que., Aug. 1982.

NUMERICAL METHODS FOR STIFF SYSTEMS OF TWO-POINT BOUNDARY VALUE PROBLEMS

Joseph E. Flaherty

and

Robert E. O'Malley, Jr.
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12181 USA

ABSTRACT

We develop numerical procedures for constructing asymptotic solutions of certain nonlinear singularly perturbed vector two-point boundary value problems having boundary layers at one or both endpoints. The asymptotic approximations are generated numerically and can either be used as is or to furnish a general purpose two-point boundary value code with an initial approximation and the nonuniform computational mesh needed for such problems. The procedures are applied to a model problem that has multiple solutions and to problems describing the deformation of a thin nonlinear elastic beam that is resting on an elastic foundation.

To appear in SIAM J. Sci. and Stat. Comput., Also NASA Contractor Report 166115, ICASE, NASA Langley Research Center, Hampton, April 1983.

ADAPTIVE FINITE ELEMENT METHODS
AND THE NUMERICAL SOLUTION OF SHEAR BAND PROBLEMS

Donald A. Drew and Joseph E. Flaherty

Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12181

ABSTRACT

Shear bands are localized regions of very high shear strain which arise as a result of high rates of loading. They occur in metal forming and cutting processes and in impact and penetration problems. In this paper, we describe a model for the formation of shear bands in simple shear that involves the description of irreversible mechanical shear and the resulting heat release. The location of a shear band is unknown in advance, and the evolution results in large gradients of displacement, velocity, and temperature. Shear band formation, therefore, offers an interesting and physically important application of a code able to resolve small-scale transient structures.

In this paper, we use an adaptive finite element code to solve several problems involving shear band formation. The code automatically locates regions with large gradients and adaptively concentrates finite elements there in order to minimize approximately the development of shear bands under many circumstances and indicate some possible mechanisms for their formation.

To appear in Phase Transitions and Material Instabilities in Solids, M. Gurtin (Ed.), Academic Press, New York, 1984.

AN ADAPTIVE LOCAL REFINEMENT FINITE ELEMENT METHOD FOR PARABOLIC PARTIAL DIFFERENTIAL EQUATIONS

Joseph E. Flaherty and Peter K. Moore

Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12181

ABSTRACT

We discuss an adaptive finite element method for solving initial-boundary value problems for vector systems of partial differential equations in one space dimension and time. The method uses piecewise bilinear rectangular space-time finite elements. For each time step, the grid is automatically refined in regions where the local discretization error is estimated as being larger than a prescribed tolerance. We discuss several aspects of our algorithm, including the tree structure that is used to represent the finite element solution and grids, an error estimation technique, and initial and boundary conditions at coarse-fine mesh interfaces. We also present the results of several computational examples and experiments.

To appear in Proc. Conf. Accuracy Estimates and Adaptive Refinements in Finite Element Computations, Lisbon, June 1984.

Numerical Integration of a Riemann Problem for a van der Waals Fluid

by

M. Slemrod

and

J. E. Flaherty

Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12181

ABSTRACT

In two recent papers Slemrod has suggested that the well known Lax-Friedrichs finite difference method may provide a natural method for the numerical integration of initial value problems with an anomalous equation of state, e.g., a van der Waals fluid. In this note we review these ideas and present the results of a numerical experiment which attempts to simulate the dynamics of a van der Waals like fluid.

Submitted to Res Mechanica, April 1984.

ON THE STABILITY OF MESH EQUIDISTRIBUTION STRATEGIES FOR TIME DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS

J. Michael Coyle, Joseph E. Flaherty and Raymond Ludwig

Department of Mathematical Sciences

Rensselaer Polytechnic Institute

Troy, New York 12181 USA

ABSTRACT

We study the stability of several mesh equidistribution schemes for time dependent partial differential equations in one space dimension. The schemes move a finite difference or finite element mesh so that a given quantity is uniform over the domain. We consider mesh moving methods that are based on solving a system of ordinary differential equations for the mesh velocities and show that many of these methods are unstable with respect to an equidistributing mesh when the partial differential system is dissipative. Using linear perturbation techniques, we are able to develop simple criteria for determining the stability of a particular method and show how to construct stable differential systems for the mesh velocities. Several examples illustrating stable and unstable mesh motions are presented.

Submitted to J. Comp. Phys., May 1984.

ON LOCAL REFINEMENT FINITE ELEMENT METHODS FOR TIME DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS

Joseph E. Flaherty
Department of Computer Science
Rensselaer Polytechnic Institute
Troy, N.Y. 12181

and

U. S. Army Armament Research and Development Command
Large Calibre Weapon Systems Laboratory
Benet Weapons Laboratory
Watervliet, NY 12189

and

Peter K. Moore
Department of Mathematical Sciences
Rensselear Polytechnic Institute
Troy, NY 12181

ABSTRACT

We discuss an adaptive finite element method for solving initial-boundary value problems for vector systems of partial differential equations in one space dimension and time. The method uses piecewise bilinear rectangular space-time finite elements. For each time step, the grid is automatically refined in regions where the local discretization error is estimated as being larger than a prescribed tolerance. We discuss several aspects of our algorithm, including the tree structure that is used to represent the finite element solution and grids, an error estimation technique, and initial and boundary conditions at coarse-fine mesh interfaces. We also present the results of several computational examples and experiments.

To appear in Proc. Second army Conf. on Appl. Maths. and Comput., R.P.I., May 1984.

A MESH MOVING TECHNIQUE FOR TIME DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS IN TWO SPACE DIMENSIONS

David C. Arney
Department of Mathematics
United States Military Academy
West Point, NY 10996
and
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, NY 12181
and
Joseph E. Flaherty
Applied Mathematics and Mechanics Section
Benet Weapons Laboratory
Watervliet, NY 12189
and
Department of Computer Science
Rensselaer Polytechnic Institute
Troy, NY 12181

ABSTRACT

We discuss an adaptive mesh moving technique that is used with a finite difference or finite element scheme to solve initial-boundary value problems for vector systems of partial differential equations in two space dimensions and time. The mesh moving technique is based on an algebraic node movement function determined from the propagation of significant error regions. The algorithm is designed to be flexible, so that it can be used with many existing finite difference or finite element methods. To test the algorithm, we implemented the mesh mover in a system code along with an initial mesh generator and a MacCormack finite volume integrator to solve hyperbolic vector systems. Results are presented for several computational examples. The moving mesh reduces dispersion erros near shocks and wave fronts and thereby can reduce the grid requirements necessary to compute accurate solutions while increasing computational efficiency.

To appear in Proc. Second Army Conf. on Appl. Maths. and Comput., R.P.I., May 1984.

A MOVING FINITE ELEMENT METHOD FOR TIME DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS WITH ERROR ESTIMATION AND REFINEMENT

by

S. Adjerid
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12181

and

J. E. Flaherty
Department of Computer Science
Rensselaer Polytechnic Institute
Troy, New York 12181

ABSTRACT

We consider a moving finite element method for vector systems of partial differential equations in one space dimension and time. The differential equations are discretized in space using a Galerkin procedure with piecewise linear approximations on a moving mesh. We simultaneously calculate an error estimation using a quadratic correction. The error estimate is used to move the mesh so that it approximately equidistributes the spatial component of the discretization error and to add and delete elements as the integration progresses. Temporal integration is performed using a stiff backward difference ordinary differential equations code. A code based on this method has been applied to several examples and their results are presented.

In preparation for SIAM J. Numer. Anal.

FOCUSING PROBLEMS FOR A NONLINEAR SCHRODINGER EQUATION

J. M. Coyle

and

Joseph E. Flaherty
Department of Mathematical Sciences
Rensselaer Polytechnic Institute
Troy, New York 12181 USA

and

Alan C. Newell
Program in Applied Mathematics
Univeristy of Arizona
Tucson, AZ 85721

ABSTRACT

We consider a cylindrically symmetric Schrodinger equation with a cubic nonlinearity. It is known that this equation has solutions that self-focus if the initial data is strong enough. We study this problem numerically using a self-adaptive finite element code and seek to determine (i) the quantitative nature of the solution as it focuses and (ii) whether the solution will still focus in the presence of a small amount of dissipation.

In preparation for Physica D.

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